Phenethyl icosanoate

Inchi: InChI=1S/C28H48O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-24-28(29)30-26-25
InchiKey: DPOBVFSNJHYUBJ-UHFFFAOYSA-N
Formula: C28H48O2
SMILES: CCCCCCCCCCCCCCCCCCCC(=O)OCCc1ccccc1
Mol. weight [g/mol]: 416.68
CAS: 608138-41-6

Physical Properties

Property code	Value	Unit	Source
gf	63.37	kJ/mol	Joback Method
hf	-629.52	kJ/mol	Joback Method
hfus	65.10	kJ/mol	Joback Method
hvap	89.35	kJ/mol	Joback Method
log10ws	-9.51		Crippen Method
logp	8.814		Crippen Method
mcvol	389.060	ml/mol	McGowan Method
pc	802.97	kPa	Joback Method
rinpol	3095.60		NIST Webbook
rinpol	3095.60		NIST Webbook
tb	943.01	K	Joback Method
tc	1155.06	K	Joback Method
tf	503.90	K	Joback Method
vc	1.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1320.09	J/mol×K	943.01	Joback Method
cpg	1410.47	J/mol×K	1119.72	Joback Method
cpg	1394.93	J/mol×K	1084.38	Joback Method
cpg	1378.20	J/mol×K	1049.03	Joback Method
cpg	1360.20	J/mol×K	1013.69	Joback Method
cpg	1340.86	J/mol×K	978.35	Joback Method
cpg	1424.89	J/mol×K	1155.06	Joback Method

dvisc	0.0000237	Pa×s	943.01	Joback Method
dvisc	0.0000319	Pa×s	869.82	Joback Method
dvisc	0.0000454	Pa×s	796.64	Joback Method
dvisc	0.0000695	Pa×s	723.45	Joback Method
dvisc	0.0001170	Pa×s	650.27	Joback Method
dvisc	0.0002249	Pa×s	577.08	Joback Method
dvisc	0.0005223	Pa×s	503.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C608138416&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume